

**PACKING POLYMORPHISM ON THE EXAMPLE OF
5-HYDROXY-1-(4-METHYLBENZYL)-3-CHLORO-4-
[(4-CHLOROPHENYL)SULFANYL]-1,5-DIHYDRO-2H-PYRROL-2-ONE:
A CRYSTALLOGRAPHIC, THERMOCHEMICAL,
AND SPECTROSCOPIC STUDY**

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Two packing polymorphs of 5-hydroxy-1-(4-methylbenzyl)-3-chloro-4-[(4-chlorophenyl)sulfanyl]-1,5-dihydro-2H-pyrrol-2-one are studied by single-crystal and powder X-ray diffraction, IR spectroscopy, and differential scanning calorimetry. Classical hydrogen bonds and Cl···O interactions have the fundamental importance for the formation of the supramolecular motif that is identical in both modifications. The difference relates to the packing of 2D layers which is “parallel” in the triclinic modification and of the “herringbone” type in the monoclinic modification. It is shown that close similarity between structural organizations of crystal lattices, which is typical of packing polymorphs, can be accompanied by significant differences between their energies as well as by a high potential barrier upon the transition from the metastable polymorph to its stable form.

DOI: 10.1134/S0022476620030142

Keywords: packing polymorphism, conformation, X-ray diffraction, crystallization, phase behavior, pyrrolinones, Cl···O interaction.

INTRODUCTION

The phenomenon of crystal polymorphism is of great importance for fundamental science, medicine, and the engineering of processes [1-5]. Currently, the following main types of polymorphism are distinguished in crystallography: conformational [2], packing [6], and synthon-based polymorphism [7]. The majority of studies are devoted to the combined conformational-synthon polymorphism, and a relatively small part of studies concern the packing polymorphism. The latter is characteristic of the substances whose molecules exhibit conformational rigidity [8, 9] and is much more seldom among conformationally mobile molecules [10, 11]. For instance, we observed on the example of a series of “flexible” chiral *para*-

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